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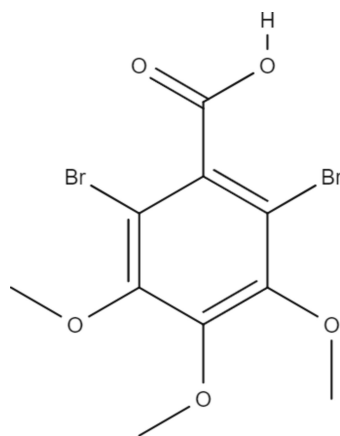
## 2,6-Dibromo-3,4,5-trimethoxybenzoic acid

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The title compound, 2,6-dibromo-3,4,5-trimethoxybenzoic acid (DBrTMBA), C<sub>10</sub>H<sub>10</sub>Br<sub>2</sub>O<sub>5</sub>, was obtained by bromination and transhalogenation of 2-iodo-3,4,5-trimethoxybenzoic acid with KBrO<sub>3</sub>. Like the previously reported 2,6-diiodo-3,4,5-trimethoxybenzoic acid (DITMBA), the structure of the title compound features a catemeric arrangement of DBrTMBA molecules along an endless chain of carboxylic H–carbonyl interactions. A short carbonyl–phenyl contact hints at a possible lone pair(O)– $\pi$ -hole interaction further stabilizing the chain-like structure over a dimeric arrangement of the carboxylic acid.

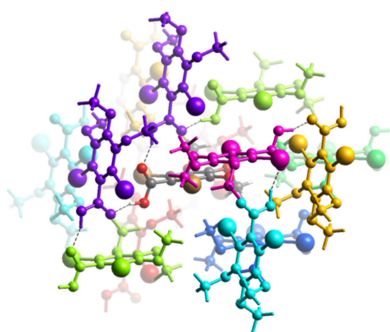
### 1. Chemical context

Organobromine compounds are valuable precursors in organic and pharmaceutical synthesis. Their participation in homo- and cross-coupling reactions is undisputed and even preferred over the other halogen-containing compounds. In practice, many brominating agents are used for their synthesis, though few of them appear to be safe both for the user-chemist and environment. Therefore, in the present work, we present a new environmentally friendly method for the synthesis of 2,6-dibromo-3,4,5-trimethoxybenzoic acid. Its structure is closely related to those of mono- and diiodo-3,4,5-trimethoxybenzoic acids ITMBA and DITMBA (Kolev *et al.*, 2021, 2023).



### 2. Structural commentary

DBrTMBA (Fig. 1) crystallizes in the monoclinic space group  $P2_1/n$  with one acid molecule in the asymmetric unit ( $Z = 4$ ). The carboxylic acid (O1/C7/O2) group is almost perpendicular to the geometrical C<sub>6</sub> mean plane and at an angle of 86.7 (2)°. This derivation is exactly in the middle of the reported geometries of the catemeric DITMBA, which is closer to 90°



**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1-H1\cdots O2^i$	0.98 (5)	1.68 (3)	2.617 (5)	160 (5)

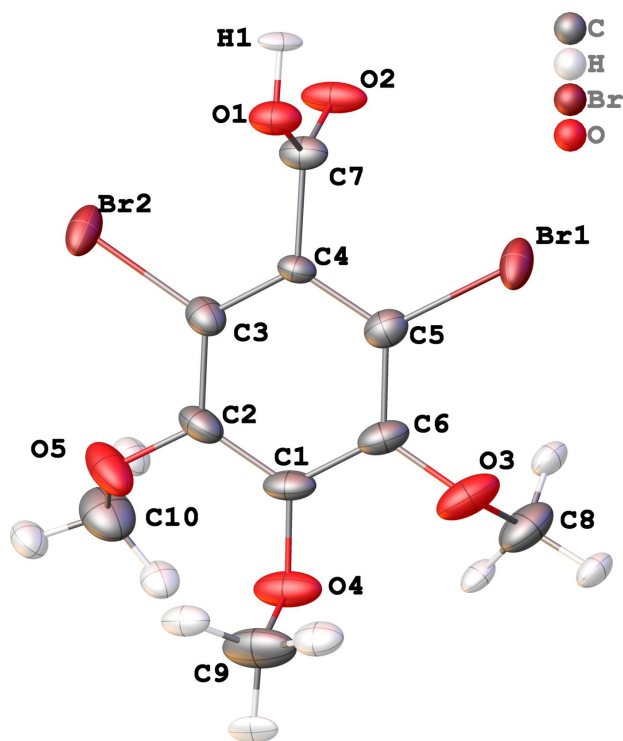
Symmetry code: (i)  $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$ .

and the reported dimeric DITMBA·toluene, which deviates more from 90° (Kolev *et al.*, 2023).

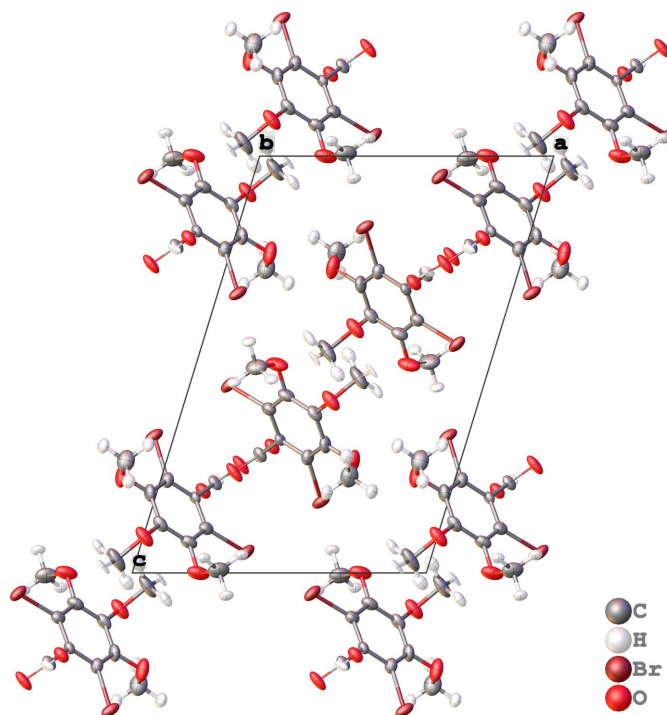
### 3. Supramolecular features

Different to the also related structures of mono- and diiodo-3,4,5-trimethoxybenzoic acids ITMBA and DITMBA·toluene (Kolev *et al.*, 2021, 2023), the title compound exhibits no dimeric structure in the solid state (Fig. 2). Instead, a hydrogen-bonded chain along the crystallographic *b*-axis direction between neighbouring acids is observed. Molecules of DBrTMBA are arranged in a catemeric fashion along this chain of carboxylic hydrogen interaction. The structure is thus very similar to that of solvent-free DITMBA (Kolev *et al.*, 2023). The O1—O2 distance of the DBrTMBA intermolecular hydrogen-bonding interaction is 2.617 (5) Å (Table 1, Fig. 3).

Another interesting structural feature in this syndiotactic arrangement can be described as a carbonyl O2 lone pair(lp)– $\pi$  ( $C_6$ ) contact with a distance from O2 to the center of geometry of the benzene ring of 3.030 (4) Å (Fig. 2). This contact presumably contributes to the deviation from the dimeric structure as observed in ITMBA and DITMBA·toluene (Kolev *et al.*, 2021, 2023). In the latter, the toluene solvent molecule seems to shield the  $C_6$   $\pi$  system from this

**Figure 1**

Labelling scheme and structure of DBrTMBA. Displacement ellipsoids are drawn at the 50% probability level.

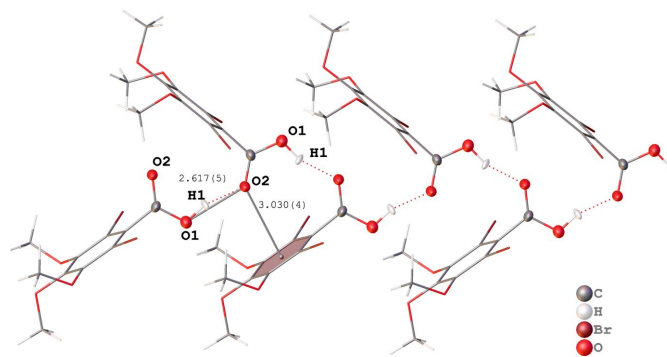
**Figure 2**

Packing of DBrTMBA along the crystallographic *b*-axis direction.

kind of interaction, giving rise to a preferred dimeric structure in this solvate.

To understand the crystal packing of DBrTMBA and the contribution of these closest interaction contacts, the software program *CrystalExplorer* was used for a Hirshfeld surface and interaction analysis (Spackman *et al.*, 2021). Fig. 4*b–d* show the closest contacts of the hydroxylic acid group as donor/acceptor in hydrogen bonding, as well as the O(lp)– $\pi$  ( $C_6$ ) interaction in Fig. 4*f*. The hydrogen donor/acceptor properties of the carboxylic group are visualized in the mapping of the electrostatic potential at the Hirshfeld surface (Fig. 4*e*).

Table 2 shows the interaction energies of DBrTMBA with the closest neighbor molecules in the crystal packing (colors in Fig. 4*g*). As expected, the strongest intermolecular interaction

**Figure 3**

Syndiotactic arrangement of DBrTMBA in the crystallographic *b*-axis direction with O(H)–O and O–center of gravity  $C_6$  and distances in Å. Atoms that are not part of the carboxylic group are shown in stick representation for clarity.

**Table 2**

Interaction Energies (kJ mol<sup>-1</sup>) for the symmetry-generated neighbors of a molecule of DBrTMBA.

Values calculated with *CrystalExplorer* at the B3LYP/6-31G(d,p) level of theory. el: electrostatic, pol: polarization, disp: energy-dispersive, rep: repulsion.

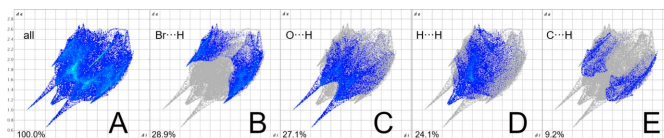
Color code	Symmetry operation	$E_{el}$	$E_{pol}$	$E_{disp}$	$E_{rep}$	$E_{total}$
Red	$-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$	-1.1	-1.0	-14.0	6.1	-10.3
Orange	$x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$	-5.6	-0.7	-10.7	8.3	-10.7
Light green	$x, y, z$	-6.3	-1.5	-25.8	16.2	-20.2
Green	$-x, -y, -z$	-3.1	-0.8	-17.3	12.9	-11.0
Cyan	$x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$	-3.3	-0.3	-7.3	8.7	-4.7
Blue	$-x, -y, -z$	-9.0	-2.0	37.6	22.1	-30.1
Purple	$-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$	-63.4	-17.1	-28.1	80.0	-54.7
Pink	$-x, -y, -z$	-1.8	-0.4	-13.8	11.4	-7.1

is exhibited over the carboxylic hydrogen contacts as well as the O(lp)- $\pi$  (C<sub>6</sub>) interaction (purple-coloured neighbors).

The fingerprint plots (Fig. 5) show the various contributions of Br···H, O···H, H···H and C···H interactions to the Hirshfeld surface, indicating a high contribution of Br···H and O···H interactions.

#### 4. Database survey

Five crystal structures from other authors featuring 3,4,5-trimethoxybenzoic acid (TMBA) are known in the Cambridge Structural Database (CSD, WebCSD search July 2023; Groom



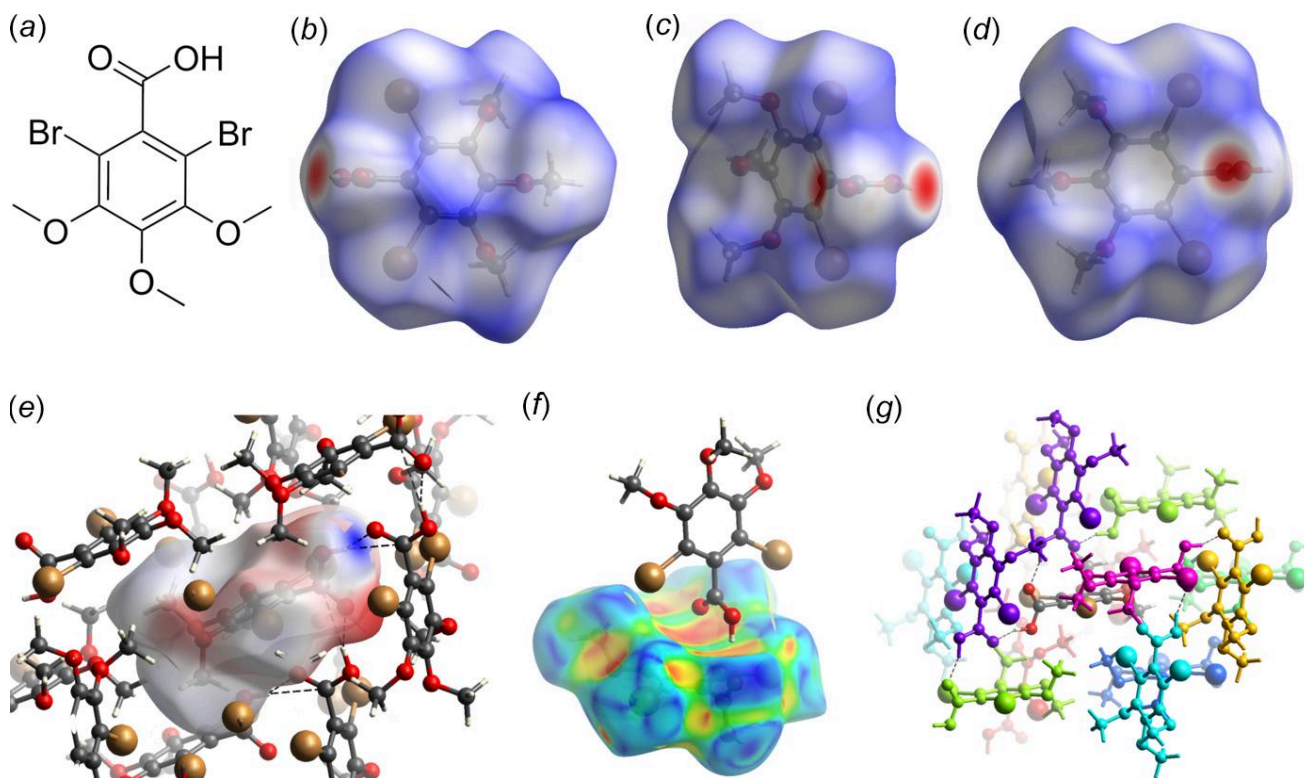
**Figure 5**

Fingerprint plots of the Hirshfeld surface of DBrTMBA.

*et al.*, 2016). The structure of the parent compound, which crystallizes in space group *Pc*, has been reported twice (Qadeer *et al.*, 2007, Bolte, 2011). Three other structures contain TMBA co-crystallized with other organic molecules (Thomas *et al.*, 2019; Chen *et al.*, 2018; Zhang *et al.*, 2021). All of them reveal co-planar arrangements of the benzene rings and hydrogen-bonding interactions. Furthermore, we recently reported on the previously discussed mono- and diiodo-3,4,5-trimethoxybenzoic acids ITMBA and DITMBA (Kolev *et al.*, 2021, 2023).

#### 5. Synthesis and crystallization

The title compound was synthesized according to the following experimental procedure: A solution of 2-iodo-3,4,5-trimethoxybenzoic acid (0.36 mmol) in 0.2 M NaOH (0.5 mL) was added dropwise to a magnetically stirred aqueous sulfuric acid solution (3.2 M, 0.6 mL) of KBrO<sub>3</sub> (0.72 mmol). The temperature of the reaction mixture was then raised gradually



**Figure 4**

Chemical scheme (a) and three different orientations (b)–(d) of the  $d_{norm}$  Hirshfeld surface of DBrTMBA. The closest contacts and the electrostatic potential [−0.077, 0.252, (e)] at the Hirshfeld surface as well as the curvature of the Hirshfeld surface (f) and overview of the nearest neighbors accompanying Table 2 (g) are depicted.

from 294 to 338 K. The resulting solution was stirred for an additional 4.0 h at 338 K and then allowed to cool slowly down (without stirring) to room temperature. The desired product, 2,6-dibromo-3,4,5-trimethoxybenzoic acid, crystallized as long, thin needles (m.p. 417–421 K; yield: 30%).

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. An Hirshfeld Atom Refinement (HAR) using *NoSpherA2* in *Olex2* was performed to obtain non-spherical atomic form factors as well as anisotropic hydrogen atomic displacement parameters (Hirshfeld, 1977, Kleemiss *et al.*, 2021). *Orca5* (Neese *et al.*, 2020) was used for the single-point calculations for the HAR procedure at def2-TZVP/M062X level of theory. The H–X distances were fixed to neutron distances from Allen & Bruno (2010) and refined anisotropically with displacement parameter restraints. The choice to fix the H–X distances to neutron distances was made because, even after several attempts at data collection, the data from DBrTMBA did not allow for the refinement of unrestrained hydrogen distances, but did allow for the refinement of softly restrained hydrogen atom anisotropic displacement parameters at these fixed distances.

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**Table 3**

Experimental details.

Crystal data	
Chemical formula	C <sub>10</sub> H <sub>10</sub> Br <sub>2</sub> O <sub>5</sub>
<i>M<sub>r</sub></i>	370.00
Crystal system, space group	Monoclinic, <i>P</i> <sub>2</sub> <sub>1</sub> / <i>n</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	11.4047 (9), 7.1107 (3), 16.8997 (13)
$\beta$ (°)	107.009 (8)
<i>V</i> (Å <sup>3</sup> )	1310.54 (16)
<i>Z</i>	4
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	6.19
Crystal size (mm)	0.08 × 0.06 × 0.03
Data collection	
Diffractometer	SuperNova, Dualflex, AtlasS2
Absorption correction	Gaussian ( <i>CrysAlis PRO</i> ; Rigaku OD, 2022)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.749, 0.855
No. of measured, independent and observed [ <i>I</i> ≥ 2 $\sigma$ ( <i>I</i> )] reflections	18764, 3245, 2254
<i>R<sub>int</sub></i>	0.084
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.667
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.053, 0.123, 1.06
No. of reflections	3245
No. of parameters	218
No. of restraints	63
H-atom treatment	Only H-atom displacement parameters refined
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	1.25, -1.48

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT2018/2* (Sheldrick, 2015), *OLEX2.refine* (Bourhis *et al.*, 2015), *NoSpherA2* (Kleemiss *et al.*, 2021), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

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## supporting information

*Acta Cryst.* (2023). E79, 916-919 [https://doi.org/10.1107/S2056989023007831]

## 2,6-Dibromo-3,4,5-trimethoxybenzoic acid

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## Computing details

Data collection: *CrysAlis PRO* 1.171.43.36a (Rigaku OD, 2022); cell refinement: *CrysAlis PRO* 1.171.43.36a (Rigaku OD, 2022); data reduction: *CrysAlis PRO* 1.171.43.36a (Rigaku OD, 2022); program(s) used to solve structure: *SHELXT2018/2* (Sheldrick, 2015); program(s) used to refine structure: *olex2.refine* 1.5-alpha (Bourhis *et al.*, 2015), *NoSpherA2* (Kleemiss *et al.*, 2021); molecular graphics: *Olex2* 1.5-alpha (Dolomanov *et al.*, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

## 2,6-Dibromo-3,4,5-trimethoxybenzoic acid

## Crystal data

$C_{10}H_{10}Br_2O_5$

$M_r = 370.00$

Monoclinic,  $P2_1/n$

$a = 11.4047$  (9) Å

$b = 7.1107$  (3) Å

$c = 16.8997$  (13) Å

$\beta = 107.009$  (8)°

$V = 1310.54$  (16) Å<sup>3</sup>

$Z = 4$

$F(000) = 718.856$

$D_x = 1.875$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 1911 reflections

$\theta = 3.1$ – $28.8$ °

$\mu = 6.19$  mm<sup>-1</sup>

$T = 100$  K

Block, clear colourless

$0.08 \times 0.06 \times 0.03$  mm

## Data collection

SuperNova, Dualflex, AtlasS2  
diffractometer

Radiation source: micro-focus sealed X-ray  
tube, SuperNova (Mo) X-ray Source

Mirror monochromator

Detector resolution: 5.2548 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: gaussian  
(*CrysAlisPro*; Rigaku OD, 2022)

$T_{\min} = 0.749$ ,  $T_{\max} = 0.855$

18764 measured reflections

3245 independent reflections

2254 reflections with  $I \geq 2\sigma(I)$

$R_{\text{int}} = 0.084$

$\theta_{\max} = 28.3$ °,  $\theta_{\min} = 3.1$ °

$h = -17 \rightarrow 19$

$k = -12 \rightarrow 6$

$l = -28 \rightarrow 28$

## Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.053$

$wR(F^2) = 0.123$

$S = 1.06$

3245 reflections

218 parameters

63 restraints

4 constraints

Primary atom site location: dual

Only H-atom displacement parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0395P)^2 + 3.4625P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.0002$

$\Delta\rho_{\max} = 1.25$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -1.48$  e Å<sup>-3</sup>

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.86638 (5)	0.67372 (7)	0.45104 (4)	0.03398 (18)
Br2	0.43161 (5)	0.68854 (7)	0.17096 (3)	0.03341 (18)
O1	0.6558 (4)	0.9831 (5)	0.3032 (2)	0.0315 (9)
H1	0.692 (6)	1.0810 (6)	0.277 (4)	0.04 (2)
O2	0.7570 (4)	0.7934 (5)	0.2410 (3)	0.0384 (11)
O3	0.7246 (5)	0.3480 (5)	0.5004 (3)	0.0468 (12)
O4	0.5037 (4)	0.1913 (5)	0.4131 (3)	0.0442 (12)
O5	0.3643 (4)	0.3576 (5)	0.2669 (3)	0.0484 (13)
C4	0.6357 (4)	0.6586 (6)	0.3198 (3)	0.0200 (10)
C5	0.7054 (5)	0.5773 (7)	0.3932 (3)	0.0278 (12)
C3	0.5234 (5)	0.5822 (7)	0.2773 (4)	0.0284 (12)
C6	0.6606 (6)	0.4204 (7)	0.4262 (3)	0.0312 (13)
C2	0.4771 (5)	0.4239 (7)	0.3079 (4)	0.0319 (13)
C7	0.6884 (5)	0.8184 (7)	0.2838 (3)	0.0261 (12)
C1	0.5451 (6)	0.3442 (7)	0.3827 (4)	0.0300 (13)
C8	0.7911 (7)	0.1815 (8)	0.4937 (4)	0.0472 (17)
H00a	0.852 (3)	0.2105 (16)	0.457 (2)	0.056 (11)
H00b	0.844 (3)	0.136 (3)	0.5545 (5)	0.057 (10)
H00c	0.7277 (7)	0.0722 (18)	0.465 (2)	0.048 (10)
C10	0.3618 (7)	0.1753 (8)	0.2314 (5)	0.0523 (19)
H00d	0.2696 (10)	0.142 (3)	0.195 (2)	0.066 (11)
H00e	0.421 (3)	0.173 (2)	0.192 (2)	0.061 (11)
H00f	0.393 (4)	0.0726 (11)	0.2799 (5)	0.060 (11)
C9	0.4330 (7)	0.2341 (9)	0.4679 (5)	0.056 (2)
H00g	0.359 (2)	0.326 (5)	0.4373 (10)	0.062 (10)
H00h	0.397 (3)	0.1060 (11)	0.485 (2)	0.052 (10)
H00i	0.4904 (11)	0.302 (5)	0.5224 (12)	0.072 (11)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Br1	0.0308 (3)	0.0207 (3)	0.0382 (4)	0.0033 (2)	-0.0091 (2)	-0.0047 (2)
Br2	0.0382 (4)	0.0181 (3)	0.0312 (3)	0.0032 (2)	-0.0097 (2)	-0.0045 (2)
O1	0.043 (2)	0.0208 (19)	0.038 (2)	-0.0014 (17)	0.0242 (19)	0.0003 (16)
H1	0.08 (4)	0.03 (3)	0.04 (3)	-0.024 (13)	0.033 (17)	-0.006 (13)
O2	0.061 (3)	0.0176 (19)	0.056 (3)	0.0006 (18)	0.047 (2)	0.0001 (18)
O3	0.083 (4)	0.029 (2)	0.031 (2)	0.010 (2)	0.021 (2)	0.0072 (18)
O4	0.068 (3)	0.021 (2)	0.062 (3)	0.0039 (19)	0.048 (3)	0.0028 (19)
O5	0.027 (2)	0.026 (2)	0.089 (4)	-0.0041 (17)	0.013 (2)	-0.007 (2)
C4	0.023 (3)	0.015 (2)	0.025 (3)	-0.0035 (19)	0.012 (2)	-0.0007 (18)
C5	0.035 (3)	0.022 (3)	0.028 (3)	0.004 (2)	0.012 (2)	0.000 (2)
C3	0.026 (3)	0.019 (3)	0.040 (3)	-0.002 (2)	0.009 (2)	-0.002 (2)
C6	0.049 (4)	0.020 (3)	0.028 (3)	0.002 (2)	0.018 (3)	0.004 (2)
C2	0.026 (3)	0.024 (3)	0.050 (4)	-0.005 (2)	0.016 (3)	-0.001 (2)
C7	0.036 (3)	0.014 (2)	0.035 (3)	0.003 (2)	0.022 (2)	-0.001 (2)

C1	0.043 (3)	0.015 (2)	0.040 (3)	-0.001 (2)	0.026 (3)	0.003 (2)
C8	0.068 (5)	0.028 (3)	0.039 (4)	0.009 (3)	0.006 (3)	0.008 (3)
H00a	0.069 (13)	0.05 (3)	0.041 (11)	0.005 (8)	0.006 (6)	0.012 (7)
H00b	0.072 (15)	0.05 (2)	0.042 (7)	0.006 (8)	0.005 (5)	0.014 (5)
H00c	0.066 (17)	0.031 (15)	0.040 (12)	0.011 (8)	0.008 (6)	0.008 (6)
C10	0.050 (5)	0.028 (3)	0.077 (6)	-0.005 (3)	0.016 (4)	-0.009 (3)
H00d	0.054 (7)	0.06 (3)	0.082 (14)	-0.012 (5)	0.015 (5)	-0.003 (8)
H00e	0.053 (10)	0.05 (3)	0.078 (13)	-0.008 (7)	0.016 (6)	-0.010 (8)
H00f	0.063 (13)	0.036 (19)	0.079 (14)	-0.003 (7)	0.018 (6)	-0.007 (8)
C9	0.076 (6)	0.036 (4)	0.081 (6)	0.010 (3)	0.063 (5)	0.010 (4)
H00g	0.082 (12)	0.038 (11)	0.09 (2)	0.012 (5)	0.059 (8)	0.008 (6)
H00h	0.081 (17)	0.033 (9)	0.073 (19)	0.012 (6)	0.070 (8)	0.003 (6)
H00i	0.10 (2)	0.041 (12)	0.092 (12)	0.008 (6)	0.051 (8)	0.007 (6)

*Geometric parameters (Å, °)*

Br1—C5	1.935 (6)	C5—C6	1.408 (7)
Br2—C3	1.948 (6)	C3—C2	1.405 (7)
O1—C7	1.299 (6)	C6—C1	1.415 (8)
O2—C7	1.224 (6)	C2—C1	1.395 (8)
O3—C6	1.354 (7)	C8—H00a	1.0770
O3—C8	1.429 (7)	C8—H00b	1.0770
O4—C1	1.346 (6)	C8—H00c	1.0770
O4—C9	1.427 (7)	C10—H00d	1.0770
O5—C2	1.355 (7)	C10—H00e	1.0770
O5—C10	1.425 (7)	C10—H00f	1.0770
C4—C5	1.388 (7)	C9—H00g	1.0770
C4—C3	1.383 (7)	C9—H00h	1.0770
C4—C7	1.496 (7)	C9—H00i	1.0770
C1—C2—C3	119.3 (5)	C8—O3—C6	113.4 (5)
C1—C2—O5	121.0 (5)	C9—O4—C1	113.8 (4)
C1—C6—C5	119.2 (5)	H00a—C8—O3	109.5
C1—C6—O3	120.2 (5)	H00b—C8—H00a	109.5
C10—O5—C2	115.5 (5)	H00b—C8—O3	109.5
C2—C1—C6	120.1 (5)	H00c—C8—H00b	109.5
C2—C1—O4	120.6 (6)	H00c—C8—H00a	109.5
C2—C3—C4	120.9 (5)	H00c—C8—O3	109.5
C2—C3—Br2	119.5 (4)	H00d—C10—O5	109.5
C3—C2—O5	119.6 (5)	H00e—C10—H00d	109.5
C3—C4—C5	120.1 (5)	H00e—C10—O5	109.5
C4—C7—O2	122.1 (4)	H00f—C10—H00e	109.5
C4—C7—O1	113.8 (4)	H00f—C10—H00d	109.5
C4—C3—Br2	119.5 (4)	H00f—C10—O5	109.5
C4—C5—Br1	121.0 (4)	H00g—C9—O4	109.5
C5—C6—O3	120.5 (6)	H00h—C9—H00g	109.5
C6—C1—O4	119.3 (5)	H00h—C9—O4	109.5
C6—C5—C4	120.3 (5)	H00i—C9—H00h	109.5

C6—C5—Br1	118.8 (4)	H00i—C9—H00g	109.5
C7—C4—C3	120.5 (5)	H00i—C9—O4	109.5
C7—C4—C5	119.1 (5)	O2—C7—O1	124.0 (5)
C7—O1—H1	109.5		
Br1—C5—C4—C3	176.9 (4)	O3—C6—C5—C4	-175.7 (5)
Br1—C5—C4—C7	2.2 (5)	O3—C6—C1—O4	-4.6 (6)
Br1—C5—C6—O3	5.3 (5)	O3—C6—C1—C2	177.3 (5)
Br1—C5—C6—C1	-177.5 (4)	O4—C1—C6—C5	178.3 (5)
Br2—C3—C4—C5	-176.2 (4)	O4—C1—C2—O5	4.4 (6)
Br2—C3—C4—C7	-1.7 (5)	O4—C1—C2—C3	-179.2 (5)
Br2—C3—C2—O5	-5.8 (5)	O5—C2—C3—C4	176.9 (5)
Br2—C3—C2—C1	177.8 (4)	O5—C2—C1—C6	-177.5 (5)
O1—C7—C4—C5	-96.1 (5)	C4—C5—C6—C1	1.4 (6)
O1—C7—C4—C3	89.3 (5)	C4—C3—C2—C1	0.5 (6)
O2—C7—C4—C5	83.0 (6)	C5—C6—C1—C2	0.2 (6)
O2—C7—C4—C3	-91.5 (6)	C3—C2—C1—C6	-1.2 (6)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1...O2 <sup>i</sup>	0.98 (5)	1.68 (3)	2.617 (5)	160 (5)

Symmetry code: (i)  $-x+3/2, y+1/2, -z+1/2$ .